Turbulent Flow and Large Surface Wave Events in the Marine Boundary Layers

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LONG-TERM GOALS

The long term objective of our research for the "High Resolution Air-Sea Interaction" (HRES) Departmental Research Initiative (DRI) is to identify the couplings between large wave events, winds, and currents in the surface layer of the marine boundary layers. Turbulence resolving large eddy simulations (LESs) and direct numerical simulations (DNSs) of the marine atmospheric boundary layer (MABL) in the presence of time and space varying wave fields will be the main tools used to elucidate wind-wave-current interactions. A suite of turbulence simulations over realistic seas using idealized and observed pressure gradients will be carried out to compliment the field observations collected in moderate to high winds. The database of simulations will be used to generate statistical moments, interrogated for coherent structures, and ultimately used to compare with HRES observations.

OBJECTIVES

Our near term goal is to participate in the planning of the HRES research initiative. This includes developing a science plan, outlining future field campaigns, and identifying opportunities for turbulence modeling studies. Also, during the planning phase of the DRI we intend to improve the parallelization of our base LES code in order to take full advantage of the modeling enhancements that will be develop as HRES evolves.

APPROACH

We plan on investigating interactions among the MABL, the ocean boundary layer (OBL), and the connecting air-sea interface using both LES and DNS. The waves will be externally imposed: (1) based on well established empirical wave spectra; or (2) ultimately provided by direct observations of the sea surface from field campaigns. The main technical advance is the development of a computational tool that allows for nearly arbitrary 3-D wave fields, *i.e.,* the sea surface elevation $\eta = \eta(x, y, t)$ as a surface boundary condition. The computational method will allow time and space varying surface conditions over a range of wave scales $\mathcal{O}(10)$m or larger.

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WORK COMPLETED

The HRES initiative is just underway and hence the work reported here falls in the category of a new start. First, in the past year we participated in the process that generated the HRES science plan; it is available from the lead authors, Professors K. Melville, C. Friehe, and D. Yue. The plan emphasizes both observations and modeling of the wave and wind fields and proposes a pilot experiment in Fall 2008 to test new instrumentation with the main experiment scheduled for Spring 2010 off the California coast. A variety of measuring platforms, *viz.,* vessels, R/P FLIP, aircraft, and buoys will be utilized in the main experiment.

In anticipation of the high-resolution computationally-intensive turbulence modeling needed for HRES, we re-visited our suite of simulation codes with the goals of improving the MPI parallelization (Message Passing Interface, Aoyama and Nakano, 1999), making the codes compliant with Fortran-90 programming practice, and adding MPI I/O (Gropp *et al.*, 1998) as the primary means of transferring data to and from disk files. Basically, the flat bottom LES code was completely re-written with the above constraints in mind. E. Patton at NCAR contributed heavily to these developments. This new code will form the baseline software which will be further modified to include the time evolving wavy lower boundary described in Sullivan *et al.*(2007).

Our previous codes use a single domain decomposition procedure that splits MPI tasks across the $z-$direction. Work is further partitioned in $x-y$ planes using a complicated mix of threaded OMP directives (Chandra *et al.*, 2001). Also, a global (elliptic) problem for pressure is solved as required for an incompressible flow. This scheme is advantageous since it does not split Fast Fourier Transforms (FFTs) across spatial directions and can utilize the architecture of machines with large numbers of CPUs per computational node (*e.g.,* the IBM SP5 with 16 CPUs/node). However the scheme falls short on other computing platforms which have few CPUs/node (*e.g.,* the Cray XT3 with 2 CPUs/node), and moreover the OMP directives require continual maintenance that adds to the code complexity. To overcome these deficiencies a new algorithm was designed based on the criteria: (1) allow arbitrary 2-D domain decomposition using solely MPI parallelization; (2) preserve pseudospectral (FFT) differencing in $x-y$ planes; and (3) maintain a Boussinesq incompressible flow model.

In the new scheme, each processor performs its operations on constricted three-dimensional bricks with the y and z directions truncated as shown in figure 1. In order to preserve pseudospectral differencing in the horizontal directions a custom MPI matrix transpose was designed and implemented. The routine performs the forward and inverse operations

$$f(x,y,z)\left[\begin{array}{ccc} & \text{all } x & \\ y_s \leq & y & \leq y_e \\ z_s \leq & z & \leq z_e \end{array}\right] \Longleftrightarrow f^T(y,x,z)\left[\begin{array}{ccc} & \text{all } y & \\ x_s \leq & x & \leq x_e \\ z_s \leq & z & \leq z_e \end{array}\right] \tag{1}$$

on the field f using a subset of horizontal processors as shown in figure 1. In (1), subscripts $(\ )_{s,e}$ denote starting and ending locations in the (x,y,z) directions. Note this transpose only requires *local* communication between processors in groups $[0-2]$, $[3-5]$, and $[6-8]$. Derivatives $\partial f/\partial y$, which are needed in physical space, are then computed in a straightforward fashion using the sequence of steps: forward x to y transpose $f \rightarrow f^T$, FFT derivative $\partial f^T/\partial y$, inverse y to x transpose $\partial f^T/\partial y \rightarrow \partial f/\partial y$. An existing serial 1-D FFT is used as in our previous codes.

The brick decomposition of the computational domain also impacts the pressure Poisson equation solver. In an incompressible Boussinesq fluid model the pressure p is a solution of the elliptic equation

$$\nabla^2 p \ = \ r\,, \tag{2}$$

where the source term r is the numerical divergence of the unsteady momentum equations (*e.g.,* see Sullivan *et al.* 1996). The solution begins with a standard forward 2-D Fourier transform of (2):

$$-\left(k_x^2 + k_y^2\right)\hat{p} + \frac{\partial^2 \hat{p}}{\partial z^2} = \hat{r}(k_y, k_x, z) \quad \text{with} \quad \left[\begin{array}{c} \text{all } k_y \\ k_{xs} \le k_x \le k_{xe} \\ z_s \le z \le z_e \end{array}\right], \tag{3}$$

where (k_x, k_y) are horizontal wavenumbers. At this stage the data layout on each processor is as shown in the upper right panel of figure 1. Custom routines carry out forward k_y to z and inverse z to k_y MPI matrix transposes on the source term of the pressure Poisson equation:

$$\hat{r}(k_y, k_x, z) \left[\begin{array}{c} \text{all } k_y \\ k_{xs} \le k_x \le k_{xe} \\ z_s \le z \le z_e \end{array}\right] \Longleftrightarrow \hat{r}^T(z, k_x, k_y) \left[\begin{array}{c} \text{all } z \\ k_{xs} \le k_x \le k_{xe} \\ k_{ys} \le k_y \le k_{ye} \end{array}\right] \tag{4}$$

The storage of $\hat{r}^T$ allows straightforward tridiagonal matrix inversion for pairs of horizontal wavenumbers on each processor; this yields the transposed field $\hat{p}^T(z, k_{xs} : k_{xe}, k_{ys} : k_{ye})$. To recover the pressure field in physical space we retrace our steps: $\hat{p}^T \rightarrow \hat{p}$ followed by an inverse 2-D Fourier transform $\hat{p} \rightarrow p$.

With these improvements the re-designed algorithm allows very large number of processors $\mathcal{O}(10^3)$ to be utilized. An important feature of the algorithm is that no global (MPI ALLTOALL) communication between processors is required. We have introduced more communication but the messages are smaller and hence large numbers of gridpoints can be used. Also, the algorithm permits the number of CPUs to exceed the number of gridpoints in the vertical direction allowing turbulent flows in large horizontal domains to be simulated.

RESULTS

In order to test the new MPI algorithm outlined above we simulated convection dominated atmospheric boundary layers (*e.g.,* Moeng 1984; Sullivan *et al.* 1998) using different meshes and brick decompositions. An illustrative example is shown in figure 2 where the mesh is $(1000 \times 1000 \times 128)$ gridpoints and the number of CPUs utilized is 128. Very large problems with 2048^3 meshes have also been run on 8192 CPUs of a Cray XT4. This new code will become the baseline code for the time evolving wavy boundary computations in HRES.

IMPACT/APPLICATIONS

The computational tool to be developed and the database of solutions that will be generated will aide in the interpretation of the observations gathered during the field campaigns of HRES. In addition idealized process studies performed with the simulations have the potential to improve parameterizations of surface drag under high wind conditions in large scale models.

TRANSITIONS & RELATED PROJECTS

We are currently engaged in analyzing data collected during the Ocean Horizontal Array Turbulence Study (OHATS) and the Coupled Boundary Layers Air-Sea Transfer (CBLAST) field campaigns. These are joint efforts between NCAR, and numerous university investigators. Also the present work has links to the future atmosphere/ocean typhoon initiatives planned by ONR.

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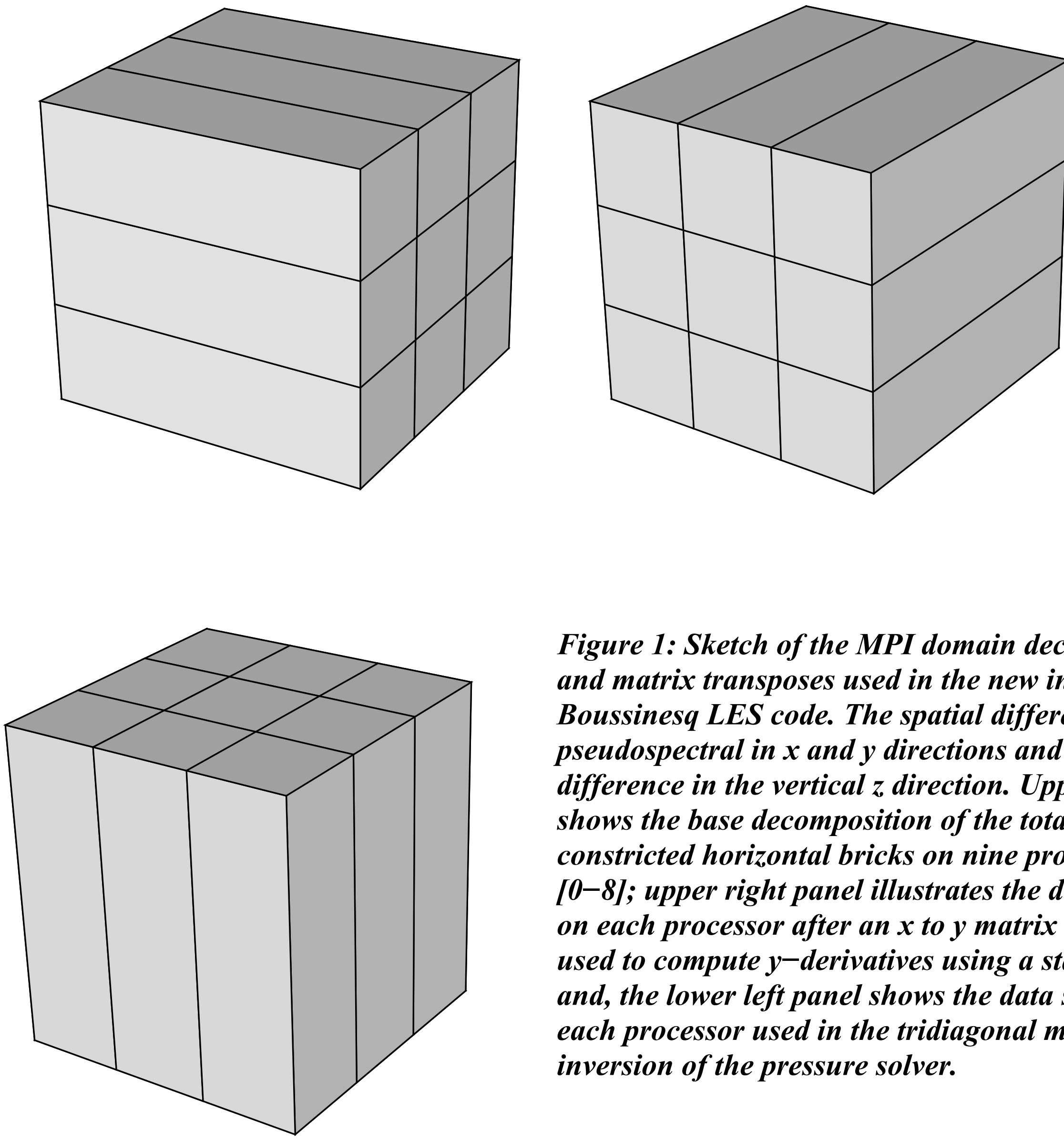

Figure 1: Sketch of the MPI domain decomposition and matrix transposes used in the new incompressible Boussinesq LES code. The spatial differencing is pseudospectral in x and y directions and finite difference in the vertical z direction. Upper left panel shows the base decomposition of the total domain into constricted horizontal bricks on nine processors [0−8]; upper right panel illustrates the data structure on each processor after an x to y matrix transpose used to compute y−derivatives using a standard FFT; and, the lower left panel shows the data structure on each processor used in the tridiagonal matrix inversion of the pressure solver.

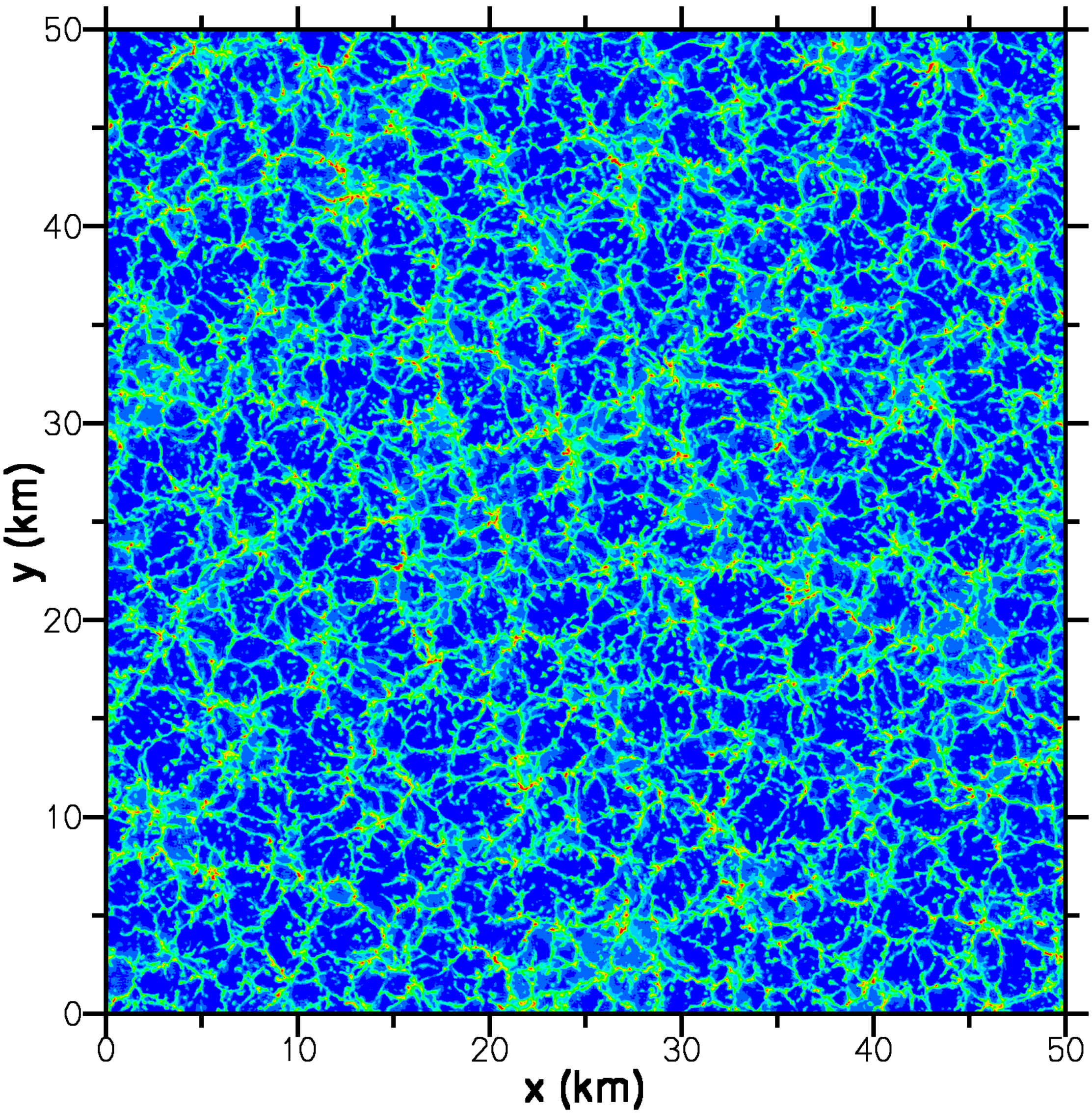

Figure 2: Visualization of potential temperature field in an $x - y$ plane at $z \sim 100$m from an LES of an atmospheric boundary layer driven by strong convection. The computational domain is near mesoscale $(50 \times 50 \times 3)$km with boundary-layer resolution $(1000 \times 1000 \times 128)$ gridpoints. The computations are done on an IBM SP5 with processor count equal to 128 CPUs. Test runs have also been carried out with meshes of 2048^3 grid points utilizing 8192 CPUs on a Cray XT4.